

STN Structure Search (Registry/Caplus)

10/518,624

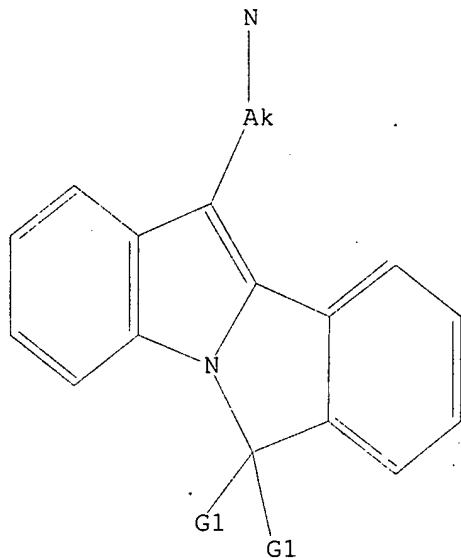
11/01/2006

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 H, Me, Et, n-Pr, i-Pr

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 18:29:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 95322 TO ITERATE

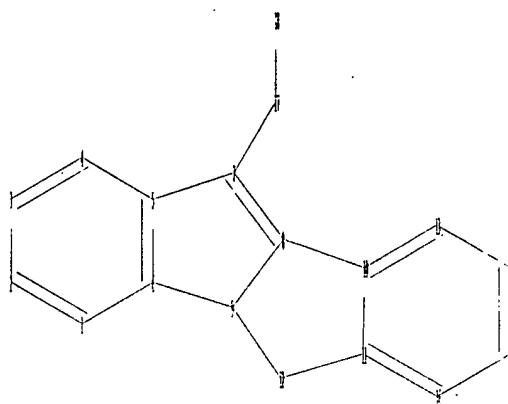
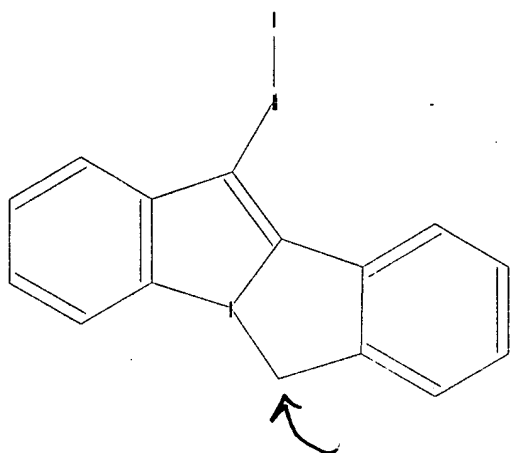
100.0% PROCESSED 95322 ITERATIONS
SEARCH TIME: 00.00.02

62 ANSWERS

L2 62 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10518624\2.str



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

ring/chain nodes :

18

chain bonds :

7-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-12 10-11 10-13 11-12
11-16 13-14 14-15 15-16

exact/norm bonds :

5-7 6-9 7-8 7-17 8-9 8-10 9-12 11-12 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-13 11-16 13-14 14-15 15-16

isolated ring systems :

containing 1 :

G1:H,CH3,Et,n-Pr,i-Pr

Match level :

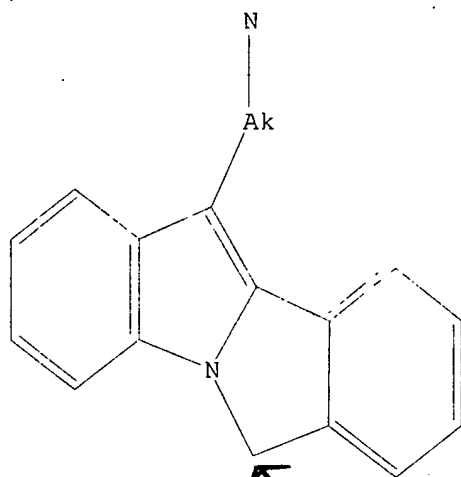
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



Gl H, Me, Et, n-Pr, i-Pr

more broad

Structure attributes must be viewed using STN Express query preparation.

=> s l3 full
 FULL SEARCH INITIATED 18:30:09 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 95322 TO ITERATE

100.0% PROCESSED 95322 ITERATIONS
 SEARCH TIME: 00.00.02

103 ANSWERS

L4 103 SEA SSS FUL L3

=> fil caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
333.88	334.09

FILE 'CAPLUS' ENTERED AT 18:30:30 ON 01 NOV 2006
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 FILE LAST UPDATED: 31 Oct 2006 (20061031/ED)

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=> s l4
L5 11 L4

=> s l2
L6 10 L2

=> d ibib abs hitstr L5 1-11

Hit # 1 - Instant

2 - 10/518,612

3-11 - all have a  group

@ R₁₃/R₁₄ or R₁₁/R₁₂ (combined)

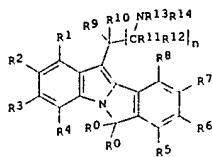
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS ON STN
 ACCESSION NUMBER: 2004:2887 CAPLUS
 DOCUMENT NUMBER: 140:77024
 TITLE: Preparation of tetracyclic arylalkyl indoles having serotonin receptor affinity
 INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadamudi
 PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India
 SOURCE: PCT Int. Appl., 66 pp.
 CODEN: PIXX2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

Instant App.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000845	A1	20031231	WO 2003-IN224	20030619
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2490115	AA	20031231	CA 2003-2490115	20030619
AU 2003249584	A1	20040106	AU 2003-249584	20030619
BR 2003012175	A	20050405	BR 2003-12175	20030619
EP 1537113	A1	20050608	EP 2003-760859	20030619
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, SI, SK, TR, LV, FI, RO, MK, CY, AL, TR, BG, SE, HU, SK			
CN 1662538	A	20050831	CN 2003-044587	20030619
JP 2006501175	T2	20060112	JP 2004-515422	20030619
US 2005203103	A1	20050915	US 2005-518624	20050513
PRIORITY APPL. INFO.:			IN 2002-MA476	A 20020621
			WO 2003-IN224	W 20030619

OTHER SOURCE(S): MARPAT 140:77024
 GI

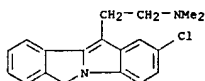
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)



AB The title compds. [I: R0 = H, alkyl; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared. Thus, reacting 1-(2'-bromobenzyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2[P(o-tolyl)3]2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indole. This invention also relates to processes for preparing the compds. 1, compns. containing effective amts. of the compound I and the use of such a compound/composition in therapy.

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L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CRN 639808-62-1
 CMF C19 H19 Cl N2



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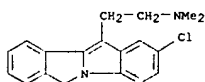
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RN 639808-67-6 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

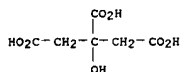
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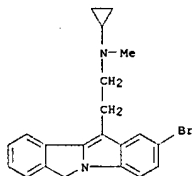


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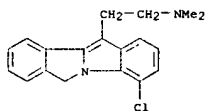
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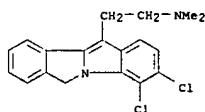
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 RN 639808-72-3 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N-cyclopropyl-N-methyl- (9CI) (CA INDEX NAME)



RN 639808-73-4 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-chloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



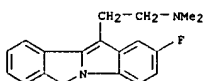
RN 639808-74-5 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3,4-dichloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



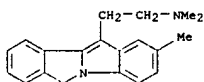
RN 639808-75-6 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 1-chloro-N,N,4-trimethyl- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

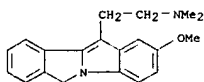
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 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-fluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



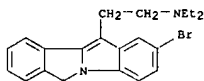
RN 639808-69-8 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N,2-trimethyl- (9CI) (CA INDEX NAME)



RN 639808-70-1 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

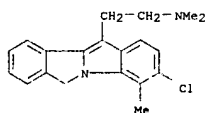
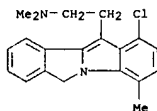


RN 639808-71-2 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-diethyl- (9CI) (CA INDEX NAME)

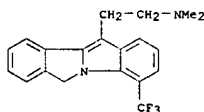


L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

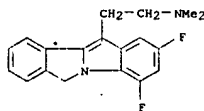
RN 639808-76-7 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,N,4-trimethyl- (9CI) (CA INDEX NAME)



RN 639808-77-8 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N-dimethyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

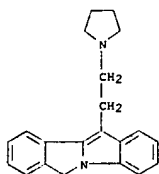


RN 639808-78-9 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2,4-difluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

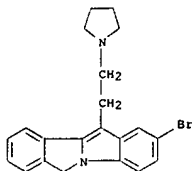


RN 639808-79-0 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole, 11-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

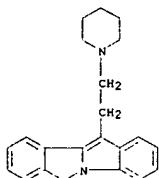
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



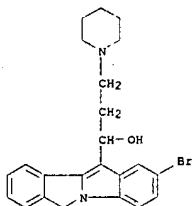
RN 639808-80-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 2-bromo-11-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)



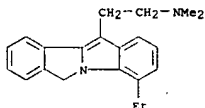
RN 639808-81-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 11-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



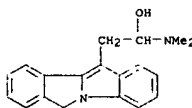
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639808-85-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)



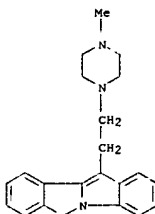
RN 639808-86-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanol, α-(dimethylamino)- (9CI) (CA INDEX NAME)



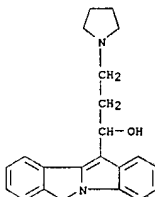
RN 639808-87-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 639808-82-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 11-[2-(4-methyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

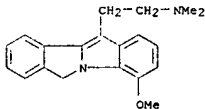


RN 639808-83-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-methanol, α-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

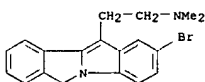


RN 639808-84-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-methanol, 2-bromo-α-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

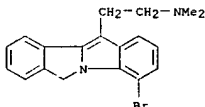
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



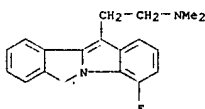
RN 639808-88-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-89-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)

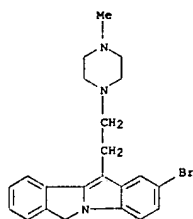


RN 639808-90-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-fluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-91-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indole, 2-bromo-11-[2-(4-methyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

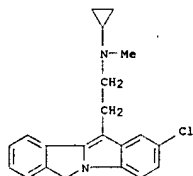
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639809-23-7 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine,
 2-chloro-N-cyclopropyl-N-methyl-
 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CM 1

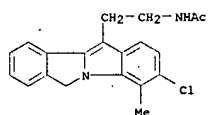
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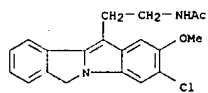
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CRN 77-92-9
 CMF C6 H8 O7

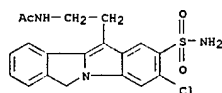
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



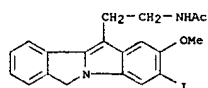
RN 639809-32-8 CAPLUS
 CN Acetamide,
 N-[2-(3-chloro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-
 (9CI) (CA INDEX NAME)



RN 639809-35-1 CAPLUS
 CN Acetamide, N-[2-[2-(aminosulfonyl)-3-chloro-6H-isoindolo[2,1-a]indol-11-yl]ethyl]- (9CI) (CA INDEX NAME)

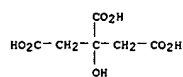


RN 639809-38-4 CAPLUS
 CN Acetamide, N-[2-(3-iodo-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-
 (9CI) (CA INDEX NAME)

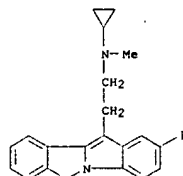


RN 639809-39-5 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,4-dimethyl- (9CI)
 (CA INDEX NAME)

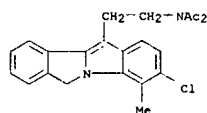
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639809-25-9 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N-cyclopropyl-2-fluoro-N-methyl-
 (9CI) (CA INDEX NAME)

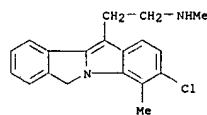


RN 639809-27-1 CAPLUS
 CN Acetamide, N-acetyl-N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

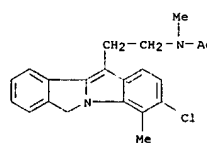


RN 639809-29-3 CAPLUS
 CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-
 (9CI) (CA INDEX NAME)

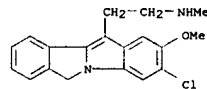
L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



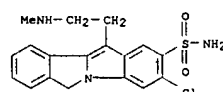
RN 639809-41-9 CAPLUS
 CN Acetamide,
 N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-
 methyl- (9CI) (CA INDEX NAME)



RN 639809-42-0 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-2-methoxy-N-methyl-
 (9CI) (CA INDEX NAME)

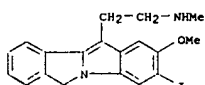


RN 639809-44-2 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639809-46-4 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-iodo-2-methoxy-N-methyl- (9CI)
 (CA INDEX NAME)

L5 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

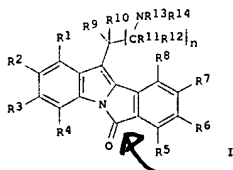
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DOCUMENT NUMBER: 140:77023
TITLE: Preparation of novel tetracyclic arylcarbonyl indoles having serotonin receptor affinity
INVENTOR(S): Jasti, Venkateswarlu; KamaKishna, Venkata Satya Nirogi; Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadiamudi
PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India; Suven Life Sciences

SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXX02
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000205	A2	20031231	WO 2003-IN223	20030619
WO 2004000205	A3	20040408		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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BR 2003012174	A	20050405	BR 2003-12174	20030619
CN 1665815	A	20050907	CN 2003-81452	20030619
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US 2005250834	A1	20051110	US 2005-518612	20050513
PRIORITY APPLN. INFO.: WO 2003-IN223 W 20030619				

OTHER SOURCE(S): MARPAT 140:77023
G1

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The title compds. [I; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared

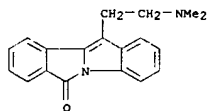
Thus, reacting 1-(2'-bromobenzoyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2[P(o-tolyl)3]2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indol-6-one. This invention also relates to processes for preparing the compds. I, compns.

containing effective amts. of the compound I and the use of such a compound/composition in therapy.

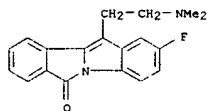
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639805-64-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoindolo[2,1-a]indolones having serotonin receptor affinity)
RN 639805-04-2 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

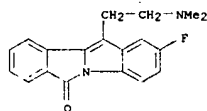
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-05-3 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)



RN 639805-06-4 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)



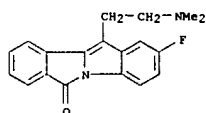
● HCl

RN 639805-07-5 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, (22)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

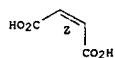
CRN 639805-05-3
CMF C19 H17 F N2 O

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



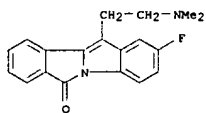
CM 2
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



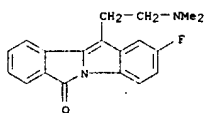
RN 639805-08-6 CAPLUS
CN Butanedioic acid, hydroxy-, compd. with 11-[2-(dimethylamino)ethyl]-2-fluoro-6H-isoindolo[2,1-a]indol-6-one (9CI) (CA INDEX NAME)

CM 1
CRN 639805-05-3
CMF C19 H17 F N2 O

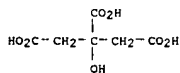


CM 2
CRN 6915-15-7
CMF C4 H6 O5

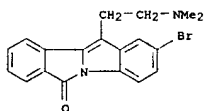
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



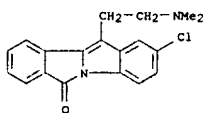
CM 2
CRN 77-92-9
CMF C6 H8 O7



RN 639805-11-1 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

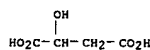


RN 639805-12-2 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 2-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



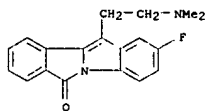
RN 639805-13-3 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 4-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-09-7 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, ethanedioate (9CI) (CA INDEX NAME)

CM 1
CRN 639805-05-3
CMF C19 H17 F N2 O



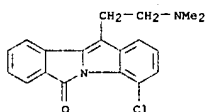
CM 2
CRN 144-62-7
CMF C2 H2 O4



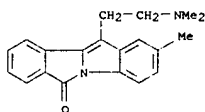
RN 639805-10-0 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CM 1
CRN 639805-05-3
CMF C19 H17 F N2 O

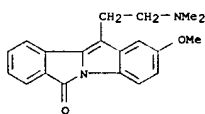
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



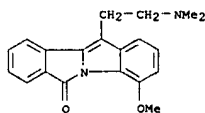
RN 639805-14-4 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methyl- (9CI) (CA INDEX NAME)



RN 639805-15-5 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methoxy- (9CI) (CA INDEX NAME)

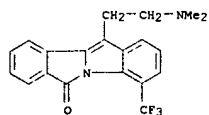


RN 639805-16-6 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methoxy- (9CI) (CA INDEX NAME)

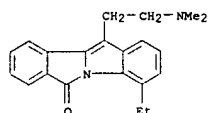


RN 639805-17-7 CAPLUS
CN 6H-isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-

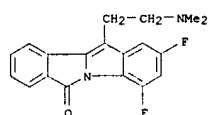
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 639805-18-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-ethyl-
(9CI) (CA INDEX NAME)



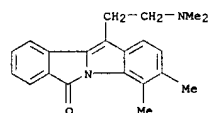
RN 639805-19-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-difluoro-
(9CI) (CA INDEX NAME)



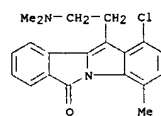
RN 639805-20-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2,4-dichloro-11-[2-(dimethylamino)ethyl]-
(9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

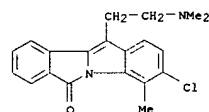
RN 639805-25-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-3,4-dimethyl-
(9CI) (CA INDEX NAME)



RN 639805-26-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1-chloro-11-[2-(dimethylamino)ethyl]-4-
methyl- (9CI) (CA INDEX NAME)

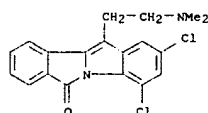


RN 639805-27-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-11-[2-(dimethylamino)ethyl]-4-
methyl- (9CI) (CA INDEX NAME)

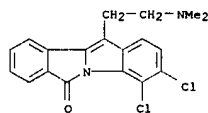


RN 639805-28-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methyl-
(9CI) (CA INDEX NAME)

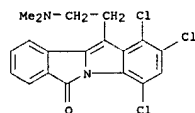
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



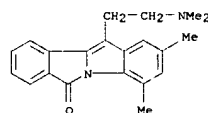
RN 639805-21-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3,4-dichloro-11-[2-(dimethylamino)ethyl]-
(9CI) (CA INDEX NAME)



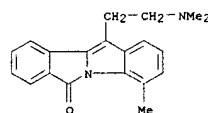
RN 639805-22-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1,2,4-trichloro-11-[2-
(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



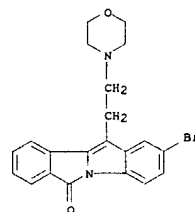
RN 639805-24-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-dimethyl-
(9CI) (CA INDEX NAME)



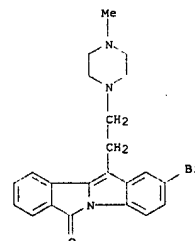
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-29-1 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(4-morpholinyl)ethyl]-
(9CI) (CA INDEX NAME)

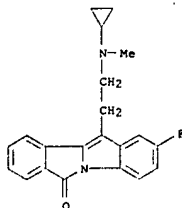


RN 639805-30-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(4-methyl-1-
piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

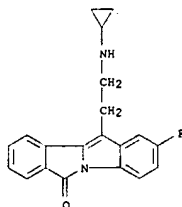


RN 639805-51-9 CAPLUS

L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylmethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

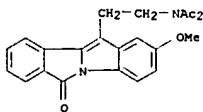


RN 639805-52-0 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

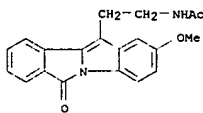


RN 639805-53-1 CAPLUS
 CN Acetamide, N-acetyl-N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

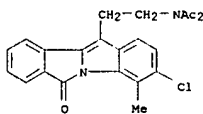
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 639805-54-2 CAPLUS
 CN Acetamide, N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

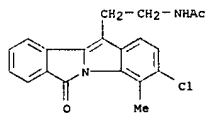


RN 639805-55-3 CAPLUS
 CN Acetamide, N-acetyl-N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

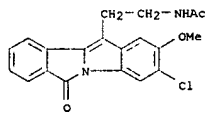


RN 639805-56-4 CAPLUS
 CN Acetamide, N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

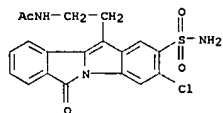
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



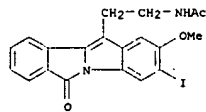
RN 639805-57-5 CAPLUS
 CN Acetamide, N-[2-(3-chloro-2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-58-6 CAPLUS
 CN Acetamide, N-[2-(2-(aminosulfonyl)-3-chloro-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

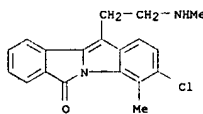


RN 639805-59-7 CAPLUS
 CN Acetamide, N-[2-(3-iodo-2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

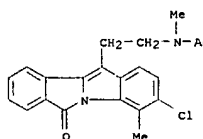


RN 639805-60-0 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-4-methyl-11-[2-

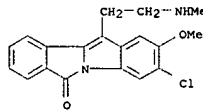
L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



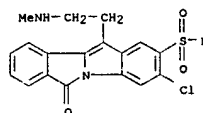
RN 639805-61-1 CAPLUS
 CN Acetamide, N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)



RN 639805-62-2 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-2-methoxy-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)

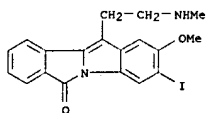


RN 639805-63-3 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-11-[2-(methylamino)ethyl]-6-oxo- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 639805-64-4 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one,
 3-iodo-2-methoxy-11-[2-(methylamino)ethyl]-
 (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:215250 CAPLUS
 DOCUMENT NUMBER: 138:362155
 TITLE: Three-Dimensional Quantitative Structure-Activity
 Relationship Studies on Selected MT1 and MT2

Melatonin Receptor Ligands: Requirements for Subtype

Selectivity

AUTHOR(S):

and Intrinsic Activity Modulation
 Rivera, Silvia; Mor, Marco; Silva, Claudia; Zuliani,
 Valentina; Vaccondio, Federica; Spadoni, Gilberto;
 Bedini, Annalisa; Tarzia, Giorgio; Lucini, Valeria;
 Pannacci, Marilou; Fraschini, Franco; Plazzi, Pier
 Vincenzo

CORPORATE SOURCE:

Dipartimento Farmaceutico, Universita degli Studi di
 Parma, Parma, I-43100, Italy

SOURCE:

Journal of Medicinal Chemistry (2003), 46(8),
 1429-1439

CODEN: JMCHAR; ISSN: 0022-2623

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The three-dimensional quant. structure-activity relation comparative mol.
 field anal. (3D-QSAR CoMFA) approach was applied to some classes of
 melatonin (MLT) membrane receptor ligands, with the principal aim of
 exploring the correlation between their steric features and MT2-selective
 antagonism. Binding data obtained from cloned MT1 and MT2 receptor
 subtypes were used to develop 3D-QSAR models for agonists and for
 antagonists at the two receptor subtypes, looking for the structural
 requirements for receptor subtype selectivity. In particular, we
 superposed the compds. showing antagonist activity, or very low intrinsic
 activity at the GTPγS test, following the hypothesis that the
 occupation of an addnl. pocket positioned out of the plane of MLT is one
 of the major determinants for MT2 selectivity; the statistical models
 obtained confirmed this hypothesis. Structure-intrinsic activity relation
 studies, applied to a set of compds. homogeneously tested, allowed the
 identification of the structural features whose modulation shifts the
 behavior from that of the agonist to that of the antagonist. The pocket
 out of the plane of MLT was identified as one of the key features for
 obtaining selective MT2 antagonists. The reliability of our statistical
 models was further confirmed by the correct prediction of the pharmacol.
 behavior of some N-substituted melatonin derivs., which were prepared and
 tested on cloned receptor subtypes.

IT

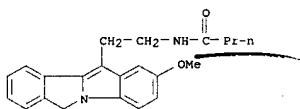
244160-10-9 263865-08-3 263865-09-4
 263865-11-8 263865-12-9 263865-13-0
 263865-14-1 263865-15-2 263865-16-3
 263865-17-4 263865-18-5 263865-19-6

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic
 use); BIOL (Biological study); USES (Uses)
 (QSAR of MT1 and MT2 melatonin receptor ligands)

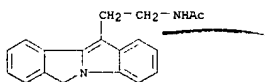
RN 244160-10-9 CAPLUS

CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
 (CA INDEX NAME)

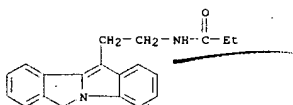
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-08-3 CAPLUS
 CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX
 NAME)

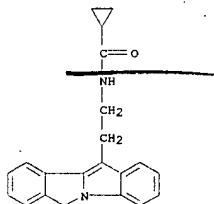


RN 263865-09-4 CAPLUS
 CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA
 INDEX NAME)

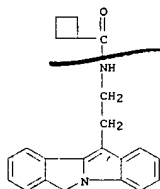


RN 263865-11-8 CAPLUS
 CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]-
 (9CI) (CA INDEX NAME)

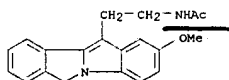
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-12-9 CAPLUS
 CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]-
 (9CI) (CA INDEX NAME)

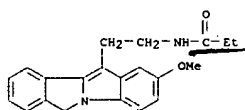


RN 263865-13-0 CAPLUS
 CN 2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
 (CA INDEX NAME)

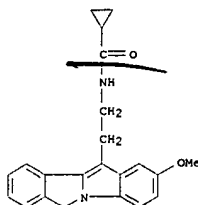


RN 263865-14-1 CAPLUS
 CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
 (CA INDEX NAME)

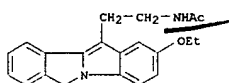
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-15-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

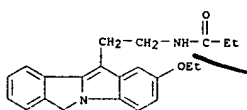


RN 263865-16-3 CAPLUS
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

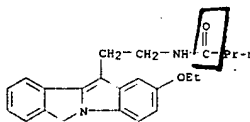


RN 263865-17-4 CAPLUS
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

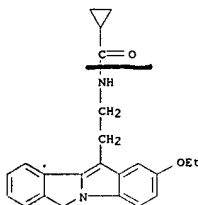
L5 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 263865-19-6 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

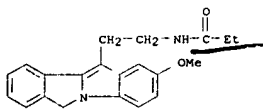
L5 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:10274 CAPLUS
DOCUMENT NUMBER: 136:64149
TITLE: 6H-Isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolines as subtype-selective melatonergics for therapeutic use
INVENTOR(S): Jones, Robert M.
PATENT ASSIGNEE(S): Cognetix, Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

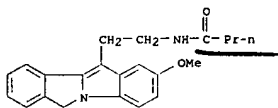
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000215	A1	20020103	WO 2001-US19958	20010622
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002040018	A1	20020404	US 2001-886609	20010622
PRIORITY APPLN. INFO.:			US 2000-304189P	P 20000623
			US 2001-264695P	P 20010130

OTHER SOURCE(S): MARPAT 136:64149
AB The invention discloses the use of MT2 selective melatonergics as anticonvulsant agents and analgesic agents. More specifically, the invention discloses the use of 6H-isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolines which have melatonin agonist activity and which are selective for the MT2 receptor as anticonvulsant agents or analgesic agents. The invention further relates to the use of 5,6-dihydroindolo[2,1-a]isoquinolines and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles which have melatonin antagonist activity and which are selective for the MT2 receptor as pharmacol. tools for delineation of physiol. responses governed by MT2 receptor activation either by melatonin or selective agonists disclosed herein and for treatment of disorders associated with overprod. of melatonin such as seasonal affective disorder (SAD) and shift work syndrome. Such melatonin antagonists are also useful for treating Parkinson's Disease.
IT 263865-14-1, CGX 031-120
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

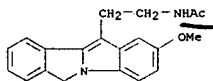
L5 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 244160-10-9, CGX 031139 263865-13-0, CGX 031133
RL: BSU (Biological study, unclassified); BIOL (Biological study) (phenylcyclidine-like behavior; isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

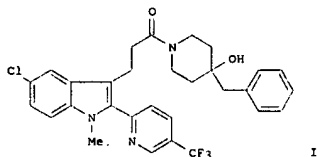


RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

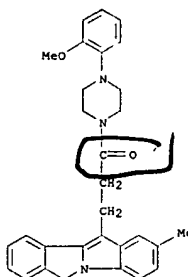
L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:321177 CAPLUS
 DOCUMENT NUMBER: 135:122368
 TITLE: 2-Aryl indole NK1 receptor antagonists: optimization of the 2-Aryl ring and the indole nitrogen substituent
 AUTHOR(S): Dinnell, K.; Chicchi, G. G.; Dhar, M. J.; Elliott, J. M.; Hollingworth, G. J.; Kurtz, M. M.; Ridgill, M. P.; Rycroft, W.; Tsao, K.-L.; Williams, A. R.; Swain, C. J.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Merck, Sharp and Dohme Research Laboratories, Neuroscience Research Centre, Harlow, Essex, CM20 2QR, UK
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(9), 1237-1240
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:122368
 GI



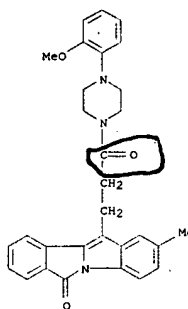
AB Novel 2-aryl indole hNK1 receptor ligands were prepared utilizing palladium cross-coupling chemical of a late intermediate as a key step. Comps. with high hNK1 receptor binding affinity and good brain penetration (e.g., I) were synthesized.
 IT 351216-15-4P 351216-16-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (optimization of the aryl ring and the indole nitrogen substituent in aryl indole NK1 receptor antagonists)
 RN 351216-15-4 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(2-methyl-6H-isoindolo[2,1-a]indol-11-yl)-1-oxopropyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L5 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

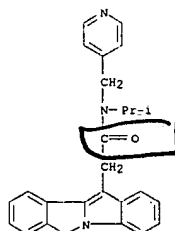


RN 351216-16-5 CAPLUS
 CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(2-methyl-6H-isoindolo[2,1-a]indol-11-yl)-1-oxopropyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:246308 CAPLUS
 DOCUMENT NUMBER: 135:70637
 TITLE: 2-Arylindole-3-acetamides FPP-Competitive inhibitors of farnesyl protein transferase
 AUTHOR(S): Trotter, B. W.; Quigley, A. G.; Lumma, W. C.; Sisko, J. T.; Walsh, E. S.; Hamann, C. S.; Robinson, R. G.; Bhinnathwala, H.; Kolodin, D. G.; Zheng, W.; Buser, A.; Huber, H. E.; Lobell, R. B.; Kohli, N. E.; Williams, T. M.; Graham, S. L.; Dinsmore, C. J.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(7), 865-869
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of 2-arylindole-3-acetamide farnesyl protein transferase inhibitors has been identified. The comps. inhibit the enzyme in a farnesyl pyrophosphate-competitive manner and are selective for farnesyl protein transferase over the related enzyme geranylgeranyltransferase-I.
 A representative member of this series of inhibitors demonstrates equal effectiveness against HDJ-2 and K-Ras farnesylation in a cell-based assay when geranylgeranylation is suppressed.
 IT 347373-82-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (arylindole acetamides farnesyl pyrophosphate-competitive inhibitors of farnesyl protein transferase)
 RN 347373-82-4 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N-(1-methylethyl)-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

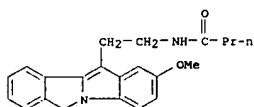
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
2000-185117 CAPLUS

DOCUMENT NUMBER: 132:273842
TITLE: Mapping the Melatonin Receptor. 6. Melatonin Agonists and Antagonists Derived from 6H-isoindolo[2,1-a]indoles, 5,6-Dihydroindolo[2,1-a]isoquinolines, and 6,7-Dihydro-5H-benzo[c]azepino[2,1-a]indoles
AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Jones, Rob; Yeh, Li-Kuan; Tsotinis, Andrew; Panoussopoulou, Maria; Calogeropoulou, Theodora; Teh, Muy-Teck; Sugden, David
CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK
SOURCE: Journal of Medicinal Chemistry (2000), 43(6), 1050-1061
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 6H-isoindolo[2,1-a]indoles, 5,6-dihydroindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human mtl and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency was measured using the pigment aggregation response of a clonal line of *Xenopus laevis* melanophores.
The 2-methoxyisoindolo[2,1-a]indoles showed much higher binding affinities than the parent isoindoles and whereas 2-methoxyisoindolo[2,1-a]indoles were agonists in the functional assay, its cyclopropanecarbonyl derivative and parent isoindoles were antagonists. The 2-ethoxyisoindolo[2,1-a]indoles showed reduced binding affinities compared to their methoxy analogs, while the 5-chloro derivative showed a considerable reduction in binding affinity and potency compared to acetyl 2-methoxyisoindolo[2,1-a]indole compound. The 10-methoxy-5,6-dihydroindolo[2,1-a]isoquinolines had higher binding affinities than the corresponding parent indoloisoquinolines in the human receptor subtypes, and the parent compds. were antagonists whereas the 10-methoxy derivs. were agonists in the functional assay. The N-cyclobutanecarbonyl derivs. of both the parent and 10-methoxy series had similar binding affinities and were both antagonists with similar potencies. The 11-methoxy-6,7-5H-benzo[c]azepino[2,1-a]indoles had higher binding affinities than the corresponding parent compds. at the MT2 receptor but similar affinities at the mtl site; all of the compds. were antagonists in the functional assay. Changing 11-methoxy for 11-ethoxy decreased the binding affinity slightly, and this was more evident at the MT2 receptor. All of the derivs. investigated had either the same or a greater affinity for the human MT2 receptor compared to the mtl receptor (range 1:1-1:132). This suggests that the mtl and MT2 receptor pockets differ in their ability to accommodate alkyl groups in the indole nitrogen

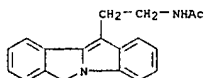
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
region of the melatonin mol. Two compds. were tested in functional assays on recombinant mtl and MT2 melatonin receptors. N-butanoyl 2-(9-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethanamine was a potent agonist with some selectivity (44-fold) for the MT2 receptor, while N-butanoyl 2-(5,6,7-trihydro-11-methoxybenzo[c]cyclohept[2,1-a]indol-13-yl)ethanamine was an MT2-preferring antagonist. Increasing the carbon chain length between N-1 of indole and the 2-Ph group from n = 1 through n = 3 leads to a fairly regular decrease in the binding affinity, but, remarkably, when n = 3, it converts the methoxy compds. from melatonin agonists to antagonists. The *Xenopus* melatonin receptor thus cannot accommodate an N-n-alkyl chain attached to a 2-Ph substituent with n > 2 in the required orientation to induce or stabilize the active receptor conformation.

IT 244160-10-9P 263865-08-3P 263865-09-4P
263865-10-7P 263865-11-8P 263865-12-9P
263865-13-0P 263865-14-1P 263865-15-2P
263865-16-3P 263865-17-4P 263865-18-5P
263865-19-6P 263865-20-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
preparation and structure of melatonin agonists and antagonists derived from isoindoloindoles, indoloisoquinolines, and benzoazepinoindoles

RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

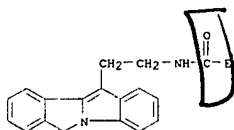


RN 263865-08-3 CAPLUS
CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

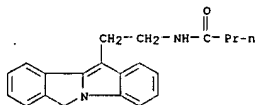


RN 263865-09-4 CAPLUS
CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

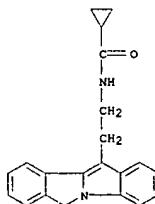
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-10-7 CAPLUS
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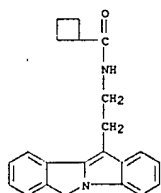


RN 263865-11-8 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

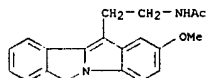


RN 263865-12-9 CAPLUS
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

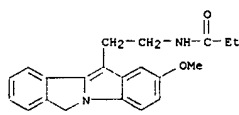
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)

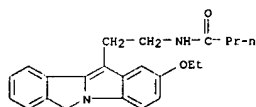


RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)

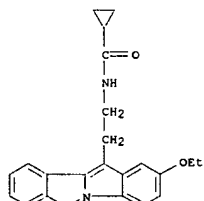


RN 263865-15-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

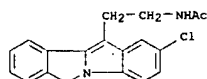
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-19-6 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

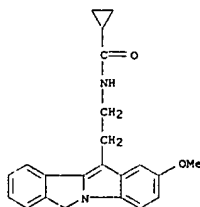


RN 263865-20-9 CAPLUS
CN Acetamide, N-[2-(2-chloro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)

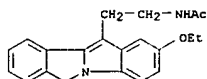


REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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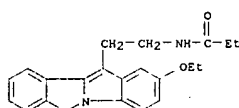
L5 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 263865-16-3 CAPLUS
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)



RN 263865-17-4 CAPLUS
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)



RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)
(CA INDEX NAME)

L5 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:442966 CAPLUS

DOCUMENT NUMBER: 131:240681

TITLE: Design of subtype selective melatonin receptor agonists and antagonists

AUTHOR(S): Sugden, David; Yeh, Li-Kuan; Teh, Muy-Teck

CORPORATE SOURCE: Physiology Division, GKT School of Biomedical Science,

SOURCE: King's College London, London, W8 7AH, UK

Reproduction, Nutrition, Development (1999), 39(3),

335-344

CODEN: RNDEES; ISSN: 0926-5287

Editions Scientifiques et Medicales Elsevier

PUBLISHER: Journal

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Studies of the physiol. actions of melatonin have been hindered by the lack of specific, potent and subtype selective agonists and antagonists. We describe the utility of a melanophore cell line from Xenopus laevis for

exploring structure-activity relationships among novel melatonin analogs and report a novel MT2-selective agonist (IIK7) and MT2-selective

receptor antagonist (K185). IIK7 is a potent melatonin receptor agonist in the melanophore model, and in NIH3T3 cells expressing human mtl and MT2

receptor subtypes. In radioligand binding expts. IIK7 is 90-fold selective for the MT2 subtype. K185 is devoid of agonist activity, but

acts as a competitive melatonin antagonist in melanophores. A low concentration (10-9M) antagonizes melatonin inhibition of forskolin stimulation of cAMP

in NIH3T3 cells expressing human MT2 receptors, but has no effect in cells expressing mtl receptors. In binding assays, K185 is 140-fold selective for the MT2 subtype.

IT 244160-10-9

RL: BAC (Biological activity or effector, except adverse); BSU

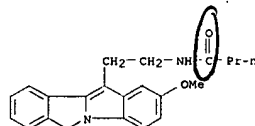
(Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(melatonin analogs structure-activity relationship in frog melanophore and human melatonin receptors)

RN 244160-10-9 CAPLUS

CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)

(CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:662000 CAPLUS

DOCUMENT NUMBER: 119:262000

TITLE: Chemistry, binding affinities, and behavioral properties of a new class of "antineophobic" mitochondrial DBI receptor complex (mDRC) ligands
 AUTHOR(S): Kozikowski, A. P.; Ma, D.; Brewer, James; Sun, S.; Costa, E.; Romeo, E.; Guidotti, A.
 CORPORATE SOURCE: Mayo Found. Med. Educ. Res., Jacksonville, FL, 32224, USA
 SOURCE: Journal of Medicinal Chemistry (1993), 36(20), 2908-20
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The mitochondrial DBI (diazepam-binding inhibitor) receptor complex (mDRC):

previously called the peripheral benzodiazepine receptors) is linked to the production of neurosteroids such as pregnenolone sulfate, dehydroepiandrosterone sulfate, and others. In order to gain further information as to the function of the mDRC in the brain, the authors have constructed and tested, both in vitro and in vivo, a novel series of ligands, 2-arylindole-3-acetamides. The SAR studies detailed herein delineate some of the structural features required for high affinity binding to the mDRCs. In most cases the new ligands were prepared by

use of the Fischer indole synthesis. Variations in the length and number of the alkyl groups on the amide nitrogen were probed together with the effects of halogen substituents on one or both of the aryl rings. Some ligands were also synthesized for study which represent conformationally constrained versions of the parent structure. Broad screening studies revealed these indoleacetamides to be highly selective for the mDRC,

since they failed to bind with any significant affinity to other receptor systems. Some of the ligands were found to exhibit Ki values in the low nanomolar range for the mDRC as measured by the displacement of [3H]4'-chlorodiazepam. A subset of these ligands was also shown to stimulate pregnenolone formation from the mitochondria of C6-2B glioma cells with an EC50 of about 3 nM. In animal expts. ligands selected for further study were found to exhibit antineophobic effects, in spite of

the fact that they exhibit no direct action on GABAA receptors.

Consequently, it is postulated that these ligands owe their action to an indirect modulation of GABAA receptor function, presumably by stimulation of neurosteroid production and release from glial cells, followed by neurosteroid modulation of GABA's action on the chloride ion channel conductance of GABAA receptors.

IT 147375-21-1P

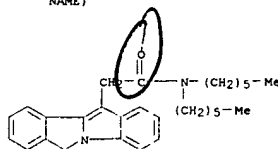
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mitochondrial diazepam-binding receptor complex

affinity of, glial neurosteroid release and GABAA receptor function modulation and antineophobic activity in relation to)

RN 147375-21-1 CAPLUS

L5 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)



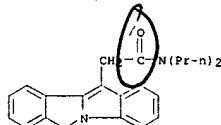
IT 135966-96-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mitochondrial diazepam-binding receptor complex

affinity of, glial neurosteroid release and GABAA receptor function modulation in relation to)

RN 135966-96-0 CAPLUS

CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:233880 CAPLUS

DOCUMENT NUMBER: 118:233880

TITLE: Preparation of indolecarboxamides and methods of treating neurological and psychiatric disorders
 INVENTOR(S): Costa, Erminio; Guidotti, Alessandro; Kozikowski, Alan; Ma, Dawei
 PATENT ASSIGNEE(S): Fidia - Georgetown Institute for the Neurosciences, USA

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

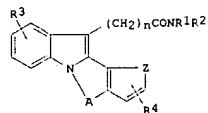
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9300334	A1	19930107	WO 1992-US5246	19920626
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CH, GA, GN, ML, MR, SN, TD, TG				
US 5206392	A	19930427	US 1991-722196	19910627
AU 9222939	A1	19930125	AU 1992-22939	19920626
EP 546164	A1	19930616	EP 1992-914902	19920626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06501030	T2	19940127	JP 1993-501593	19920626
PRIORITY APPLN. INFO.: US 1991-722196 A 19910627				
WO 1992-US5246 A 19920626				

OTHER SOURCE(S): MARPAT 118:233880

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AB Title compds. I (R1, R2 = H, C3-12 alkyl, (alkyl)aryl; R1R2 = 4-6-membered

(un)saturated ring; R3, R4 = H, C1-12 alkyl, O2N, H2N, N3, cyano, halo, RO2C,

RO, RS (wherein R = H, alkyl); A = C1-3 alkylene to form a ring or null;

Z = O, NH, S, CH:CH; n = 1-3) or their salts are prepared PhNHNH2, PhCOCH2CH2CO2H and H2SO4 in EtOH were refluxed for 24 h, cooled and

extracted with Et2O to give Et 2-phenyl-3-indoleacetate which in 3N NaOH was refluxed for 3 h, acidified with HCl and treated with Me(CH2)5NH2, PhOP(O)(Cl)NHPh, and Et3N to give I (A = null, Z = CH:CH, R1 = R3 = R4 = H, R2 = hexyl, n = 1). I showed anxiolytic action in rodents at 0.1-0.5

L5 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

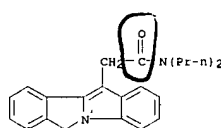
mg/kg.

IT 135966-96-0P 147375-21-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as drug for treatment of neurol. disorders and as

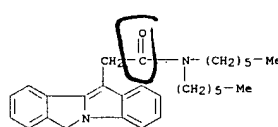
RN 135966-96-0 CAPLUS

CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



RN 147375-21-1 CAPLUS

CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)



L5 . ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1991:535868 CAPLUS
 DOCUMENT NUMBER: 115:135868
 TITLE: Palladium catalyzed synthesis of annelated indoles
 AUTHOR(S): Kozikowski, Alan P.; Ma, Dawei
 CORPORATE SOURCE: Mayo Clin., Jacksonville, FL, 32224, USA
 SOURCE: Tetrahedron Letters (1991), 32(28), 3317-20
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 115:135868
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of polycyclic indoles, e.g., I (X = O, CH₂), II, III, is shown to be accomplished readily by the palladium catalyzed intramolecular cyclization of bromoarylindoles, e.g., IV, V, VI.

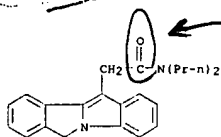
IT 135966-96-0P

RJ: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 135966-96-0 CAPLUS

CN 6H-Indolo[2,1-b]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)

same as #10



R₁₁ R₁₂

are acyl